# Fermions in 2D Optical Lattices: Temperature and Entropy Scales for Observing Antiferromagnetism and Superfluidity

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One of the major challenges in realizing antiferromagnetic and superfluid phases in optical lattices is the ability to cool fermions. We determine constraints on the entropy for observing these phases in two-dimensional Hubbard models. We investigate antiferromagnetic correlations in the repulsive model at half filling and superfluidity of s-wave pairs in the attractive case away from half filling using determinantal quantum Monte Carlo simulations that are free of the fermion sign problem. We find that an entropy per particle $\simeq \ln 2$ is sufficient to observe the charge gap in the repulsive Hubbard model or the pairing pseudogap in the attractive case. Observing antiferromagnetic correlations or superfluidity in 2D systems requires a further reduction in entropy by a factor of three or more. In contrast to higher dimensions, we find that adiabatic cooling is not useful to achieve the required low temperatures. We also show that double occupancy measurements are useful for thermometry for temperatures greater than the nearest-neighbor hopping.

An exciting new development in cold atoms is the ability to realize in the laboratory simple models of strongly correlated fermions in optical lattices [1, 2, 3, 4, 5, 6]. These studies are motivated by their relevance to spectacular phenomena in condensed matter physics, like high $T_c$ superconductivity, that are not fully understood. The best known model is the fermion Hubbard Hamiltonian[7, 8] that captures the physics of antiferromagnetism and, at least qualitatively, d-wave superconductivity in two dimensions (2D). The Hubbard model is well understood in one dimension (1D), using exact solutions and bosonization [9], and also in the limit of large dimensions, using dynamical mean field theory (DMFT) [10]. The *two dimensional* problem, of direct relevance to layered high $T_c$ superconductors, is the least well understood theoretically. New insights into the 2D Hubbard model can come from cold atom emulators, given their high degree of tunability (interaction strength, chemical potential) and absence of disorder and material complications.

The principal challenges for the optical lattice emulators are to cool down to sufficiently low temperature to see interesting phases and to observe the characteristic order. In this paper we present detailed quantitative results from quantum Monte Carlo (QMC) simulations [7] of (i) the 2D repulsive ($U > 0$) Hubbard model at half filling and (ii) the 2D attractive ($U < 0$) Hubbard model at any filling, that are both of direct relevance to ongoing experiments. The reasons for focusing on these systems are threefold. Determinantal QMC simulations are free of the fermion "sign problem" [11] in both cases and we can obtain non-perturbative results on finite systems without any approximations. These two systems exhibit phenomena of great interest: strong antiferromagnetic correlations and Mott physics for $U > 0$, and a

Berezinskii-Kosterlitz-Thouless (BKT) transition to an s-wave superfluid [12] with a pairing pseudogap [13] above $T_c$ for $U < 0$. Finally, both these models are realizable in cold atom systems where, e.g., a Feshbach resonance can be used to change the sign of the interaction.

Our main results are: (1) we determine the characteristic temperature scales for spin, charge and pairing correlations and the superfluid $T_c$ as functions of the interaction strength. (2) We determine constant entropy contours in the temperature-interaction plane, that give direct information on how much the system has to be cooled, i.e., how low the entropy should be in the experiments, in order to see interesting physics. (3) We comment on the difficulty of using adiabatic cooling in 2D. (4) Finally we point out the temperature range in which a simple observable like double occupancy can be used for thermometry.

The single band Hubbard Hamiltonian is

$$
\begin{aligned}
\mathcal{H} &= -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) \\
&+ U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) - \mu \sum_i n_i \qquad (1)
\end{aligned}
$$

where $c_{i\sigma}$ is the fermion destruction operator at site $i$ with spin $\sigma$, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the density of fermions with spin $\sigma$, and $n_i = \sum_\sigma n_{i\sigma}$. For cold atoms $\sigma = \uparrow, \downarrow$ labels two hyperfine states. We consider near-neighbor hopping on a square lattice with the kinetic energy $\epsilon(\mathbf{k}) = -2t(\cos k_x a + \cos k_y a)$. In the determinantal QMC calculation, we work in the grand canonical ensemble and tune the chemical potential $\mu$ to obtain the desired density $\rho = \sum_i \langle n_i \rangle / N$ on an $N$-site lattice. The parameters $t$ and $U$ can be directly related [6] to the lattice depth $V_0$, tuned by the laser intensity, and to the interatomic interaction tuned by a Feshbach resonance. We work in a
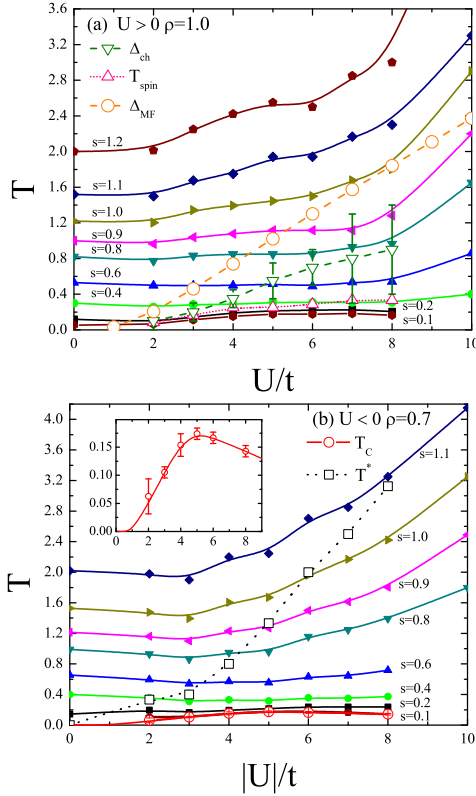
FIG. 1: Phase diagrams of the 2D Hubbard Models with (a) repulsive ($U > 0$) interactions at half filling and (b) attractive ($U < 0$) interactions away from half-filling, showing curves of constant entropy (per site) $s = S/Nk_B$, obtained from QMC simulations on $N = 10^2$ lattices. In (a) $\Delta_{\mathrm{ch}}$ is the scale for the formation of a charge gap, $\Delta_{\mathrm{MF}}$ is the mean field charge gap (see text), and $T_{\mathrm{spin}}$ is obtained from the peak in $\chi(T)$ in Fig. 2(b). In (b), the pairing pseudogap temperature $T^*$ is obtained from the peak in $\chi(T)$ in Fig. 2(c), and the Berezinskii-Kosterlitz-Thouless transition $T_c$ is estimated from the superfluid density, Fig. 2(d); $T_c$ as a function of $U$ also shown in the inset.

parameter regime where only a single band is populated in the optical lattice. All energies and temperatures are measured in units of $t$ and distances in units of $a$.

The results for the characteristic temperature scales (open symbols) and constant entropy curves (filled symbols) in the $(T, U)$-plane are shown in Fig. 1. We first describe the results for the repulsive ($U > 0$) model at half-filling $\rho = 1$ and then turn to the attractive ($U < 0$) case at arbitrary filling $\rho \neq 1$.

**Repulsive Hubbard model at half-filling:** Coming down from high temperatures the first scale encountered is the energy gap to charge excitations. A lower scale corresponds to the development of spin correlations. The Mermin-Wagner theorem precludes a finite temperature phase transition in this 2D system and both these scales are crossovers. Nevertheless, these scales (summarized in Fig. 1) have very clear signatures in physical observables (Figs. 2,3,4).

Charge gap: The charge gap is seen in Fig. 2(a) where

we plot the density $\rho$ as a function of the chemical potential $\mu$. Despite large error bars, arising from the sign problem *away* from half-filling, we clearly see that the compressibility $d\rho/d\mu$ is very small; it should vanish at $T = 0$. The region $|\mu| < \Delta_{\mathrm{ch}}$ for which $d\rho/d\mu \approx 0$ gives an estimate of the charge gap $\Delta_{\mathrm{ch}}$. The $U/t$-dependence of the charge gap is shown in Fig. 1(a): for $T \gg \Delta_{\mathrm{ch}}$ we expect the system to look effectively gapless while for $T \ll \Delta_{\mathrm{ch}}$ there is a gap to fermionic excitations.

For large $U$ the charge gap scales linearly with $U$ and is called the Mott gap, but it becomes (exponentially) small for low $U$. To understand this $U$-dependence we use a simple $T = 0$ mean field theory (MFT) of spin density wave (SDW) ordering that shows the system is an insulator at $\rho = 1$ for any $U > 0$. The $U = 0$ metal is unstable due to Fermi surface nesting, and the ground state is an insulator whose gap is obtained from $N^{-1} \sum_{\mathbf{k}} [\epsilon_k^2 + \Delta_{\mathrm{MF}}^2]^{-1/2} = 1/U$. The mean field charge gap is $\Delta_{\mathrm{MF}} \sim t \exp{-2\pi\sqrt{t/U}}$ for $U/t \ll 1$ and smoothly crosses over to the Mott gap $\Delta_{\mathrm{MF}} = U/2$ for $U/t \gg 1$. This evolution [14] from a SDW insulator to a Mott insulator is the $U > 0$ analog of the BCS to BEC crossover in attractive Fermi systems. We see from Fig. 1(a) that the $U/t$-dependence of $\Delta_{\mathrm{MF}}$ obtained from $T = 0$ MFT overestimates the charge gap obtained from the $\rho(\mu)$ analysis for moderate to large coupling. The MFT is also quite misleading about the finite temperature antiferromagnetic (AF) long range order, that is necessarily absent in 2D.

Spin correlations: To study magnetic correlations we look at the uniform susceptibility $\chi(T)$ for various $U/t$ shown in Fig. 2(b). We find a broad peak in $\chi(T)$ at a temperature $T_{\mathrm{spin}}$ below which short range AF spin correlations are important. We have also analyzed the short range spin-spin correlation function $\langle S_i \cdot S_{i+\delta} \rangle$ as a function of $T$ for various $U/t$ and found that it too shows a growth in correlations at the temperature scale $T_{\mathrm{spin}}$.

To get a better feel for $T_{\mathrm{spin}}$ we also plot in Fig. 2(b) the uniform susceptibility for the 2D nearest-neighbor $S = 1/2$ Heisenberg AF [15], that describes the low energy spin physics of the Hubbard model for $U/t \gg 1$. Here we see a peak in $\chi$ at $T_{\mathrm{spin}} = J_{\mathrm{AF}}$. To plot this data together with our Hubbard model results, we have chosen (somewhat arbitrarily) $U/t = 12$, so that the AF superexchange $J_{\mathrm{AF}} = 4t^2/U = t/3$.

Except in weak coupling $U/t \ll 1$, where the charge and spin scales are essentially identical, we find in Fig. 1(a) that the two scales are quite different for $U/t > 1$. In the large $U$ (Mott) limit we expect $\Delta_{\mathrm{ch}} = U/2 \gg T_{\mathrm{spin}} \simeq J_{\mathrm{AF}} = 4t^2/U$. For any $U/t$ we expect to see local moments below the charge gap $T < \Delta_{\mathrm{ch}}$, and the build up of AF spin correlations between the moments for $T < T_{\mathrm{spin}}$.

Entropy: In cold atom experiments the entropy $S$ can be monitored more easily than the temperature. We calculate $S(T)$ from QMC in two different ways. The
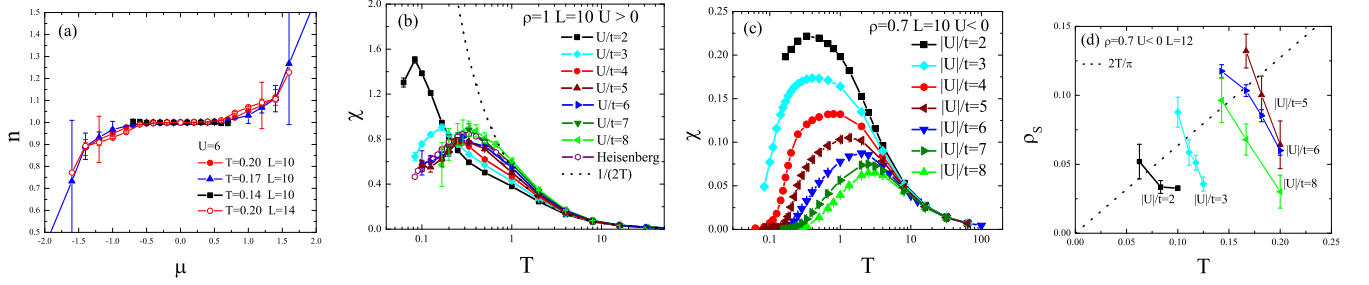
FIG. 2: (a) Density $\rho$ as a function of chemical potential $\mu$ for $U = 6t$ and various $T$. Note that $\rho$ is pinned at unity for $|\mu| \leq \Delta_{\text{ch}}$, the charge gap. The large error bars away from half-filling are a result of the sign problem. Spin susceptibility $\chi(T)$ for (b) positive $U$ at half filling and (c) negative $U$ at density $\rho = 0.7$. The peak in $\chi(T)$ is used to determine characteristic temperature scales for the two models described in the text. (d) The superfluid density $\rho_s(T)$ for various $U < 0$ at $\rho = 0.7$. This is used to estimate the Kosterlitz-Thouless $T_c$ in 2D using $\rho_s(T_c) = (2/\pi)T$.
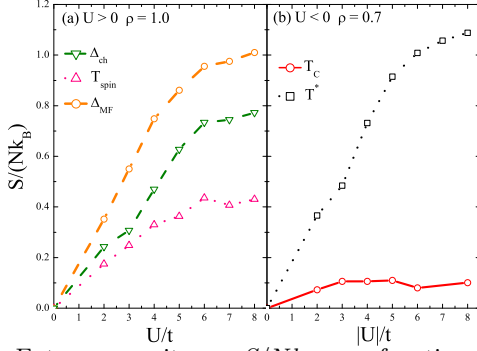


FIG. 3: Entropy per site $s = S/Nk_B$ as a function of $U$ at a temperature corresponding to the characteristic scale for that $U$. (a) For $U > 0$, the entropy at $\Delta_{\text{ch}}$, the charge scale, and $T_{\text{spin}}$, the spin scale is plotted. (b) For $U < 0$ the entropy at the pairing scale $T = T^*$ and the superfluid $T = T_c$ is plotted.

first method [16, 17] is to integrate down from infinite temperatures: $S(\beta) = \rho N \ln 4 + \beta E(\beta) - \int_0^\beta d\beta' E(\beta')$, where $\beta = 1/T$ and $E$ is the energy. The second method [18] is to integrate up from $T = 0$. Here we fit $E(T)$ data to a suitable functional form, find the specific heat $C(T) = dE(T)/dT$ and calculate $S(T) = \int_0^T C(T')/T'$. The methods agree to within a few percent.

The curves of constant $S$ are plotted in the $(U,T)$-plane in Fig. 1(a). At weak coupling the charge and spin scales are both exponentially small and the system looks like a highly degenerate normal Fermi gas with a low entropy. It is only at very low entropy (per particle) $s \ll \ln 4 \simeq 1.386$, that one observes either the charge gap or build up of spin correlations for $U/t \leq 1$. For moderate coupling, say, $U/t \simeq 6$ we see that $s = \ln 2 \simeq 0.693$ already puts us below the charge gap scale. By lowering the entropy to $s \sim 0.4$ it is already possible to cross $T_{\text{spin}}$. The difference between the entropy required to access the charge and spin scales grows as $U$ increases. We note that $T_{\text{spin}}$ sets the maximum scale for the AF $T_{\text{Neel}}$ if we were to couple 2D layers to cut off the fluctuations and stabilize AF order in layered system like the parent insulator of the high Tc superconductor. In Fig. 3, we summarize our results for the entropy per site $S/Nk_B$ at the charge and spin temperature scales plotted as function of $U$.
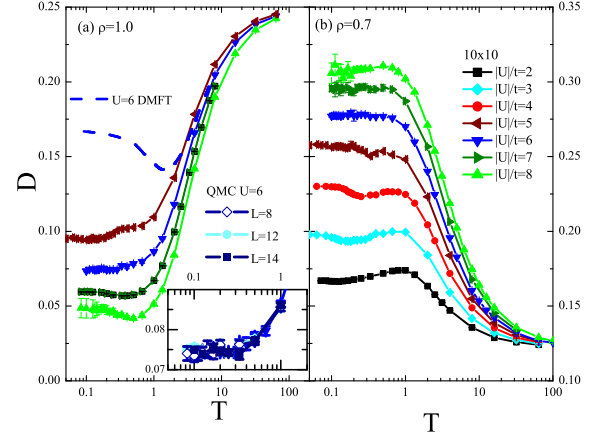


FIG. 4: Double occupancy $\langle n_{i\uparrow}n_{i\downarrow}\rangle$ as a function of temperature $T$ for (a) $U > 0$ and (b) $U < 0$. The legend in (b) also apply to the positive $U$ values in (a). Also shown are the comparisons with dynamical mean field theory DMFT in panel (a) that shows a much more pronounced anomalous region with $dD/dT < 0$. The inset in (a) shows the lack of system size dependence in the $D(T)$ results.

Cooling and Thermometry: We next turn to a beautiful suggestion of Werner *et. al.* [19] for adiabatic cooling in an optical lattice, that exploits the anomalous $T$-dependence of the double occupancy $D = \langle n_{i\uparrow}n_{i\downarrow}\rangle$ observed in dynamical mean field theory (DMFT). In brief, their idea is as follows. The entropy and $D$ are related to the free energy $F$ via $S = -\partial F/\partial T$ and $D = \partial F/\partial U$. Using a Maxwell relation we find $\partial S/\partial U = -\partial D/\partial T$. For $U > 0$, the "natural" expectation is $dD/dT > 0$ so that the temperature increases along a constant $S$ curve upon increasing $U/t$. Thus the DMFT observation of a significant anomalous region with $dD/dT < 0$ implies that we can follow a curve of constant $S$ and cool the system as the lattice is turned on, i.e., $U/t$ is increased.

We show in Fig. 4(a) the DMFT curve for $D(T)$ at $U = 6t$ contrasted with 2D QMC results. The absence of a significant anomalous regime with $dD/dT < 0$ in 2D is likely a result of short range spin correlations that are important in low dimensional systems but neglected in DMFT. We see that the constant-$S$ curves in Fig. 1(a) do not show a significant negative slope and thus one

cannot obtain adiabatic cooling in 2D.

From Fig. 4(a) we see that the double occupancy $D(T)$ is quite weakly $T$-dependent for $T < t$, but its monotonic $T$-dependence at higher temperature suggests that $D(T)$, that can be measured in cold atom experiments [3], can be used for thermometry in the range $1 < T/t < 10$. Such a thermometer would need QMC results for $D(T)$ callibration. We show in the insert to Fig. 4(a) that the double-occupancy, that is a local observable, has no significant system size dependence and can indeed be very accurately determined by QMC.

**Attractive Hubbard model at arbitrary filling:** The $U > 0$ model away from $\rho = 1$ has a fermion sign problem in QMC, so we turn to a different model to discuss superfluidity in a 2D lattice system. We change the sign of the interaction and examine the attractive Hubbard model that exhibits s-wave pairing [12] and a BCS to BEC crossover [13] as a function of $|U|/t$. We will consider the case of $\rho = 0.7$ filling for concreteness; we choose to work away from half-filling, because at $\rho = 1$ the results would be identical to those discussed above using a well-known particle-hole transformation.

Pairing (Pseudogap) scale: The analog of the charge scale below which moments form in the repulsive model, is the pairing scale $T^*$ in the attractive Hubbard model below which double occupancy grows. Since pairing represents the onset of singlet correlations, one of the simplest ways of probing this scale is through the susceptibility $\chi(T)$ plotted in Fig. 2(c) for a sequence of attractive couplings $|U|/t$. The peak in $\chi$ is a measure of the pairing scale, for below it the spin response is strongly suppressed by the formation of pairs. The $|U|/t$-dependence of $T^*$ as determined from $\chi$ is plotted in Fig. 1(b). $T^*$ essentially has the same $|U|$-dependence as the $T = 0$ pairing gap: exponentially small in $|U|/t$ for the weak coupling BCS limit and proportional to $U$ in the strong coupling Bose limit. For $T < T^*$ there is a pseudogap [13] due to pairing correlations in the density of states, even above $T_c$ where the system is not superfluid.

Berezinskii-Kosterlitz-Thouless Transition: At lower temperatures there is a transition to a superfluid phase in the attractive Hubbard model for $\rho \neq 1$. There is algebraic order in the pair-pair correlation function [12] below $T_c$ and a non-zero superfluid density $\rho_s$. We calculate $\rho_s$ from the transverse current-current correlation function [20] and use the universal jump in $\rho_s(T_c^-) = 2T_c/\pi$ to estimate the BKT $T_c$ as shown in Fig. 2(d). At a filling of $\rho = 0.7$ there is a maximum in $T_c \simeq 0.2t$ as a function of attraction at $|U|/t \simeq 5$ as seen from Fig. 2(d). The non-monotonic dependence of $T_c$ on $|U|/t$ is expected with an exponentially small $T_c$ in the weak coupling BCS limit and $T_c \sim t^2/|U|$ in the strong coupling BEC limit.

Entropy, Cooling and Thermometry: We next calculate the entropy using the methodology described above and plot the curves of constant $S$ in the $(|U|, T)$-plane in Fig. 1(b). We see from Figs. 1(b) and 3(b) that for a coupling $|U|/t \simeq 5$ at which the $T_c$ peaks for $\rho = 0.7$, one only needs to lower the entropy $S/Nk_B < 0.8$ to enter the pseudogap regime below $T^*$. To actually observe superfluidity one needs to cool below the BKT transition, that corresponds to $S/Nk_B < 0.1$.

The double occupancy $D(T)$ for $U < 0$ in Fig. 4(b) shows a rather small regime of anomalous behavior, which now corresponds to $dD/dT > 0$. Thus the prospects of using adiabatic cooling [19] in 2D do not look promising for the attractive case either. However, Fig. 4(b) does suggest that $D(T)$ can be used as an effective thermometer for the high temperature range $t < T < 10t$.

**Conclusions:** Current fermion optical lattice experiments [4] have achieved an entropy per particle $\simeq \ln 2$, sufficient to observe the charge gap in the repulsive Hubbard model or the pairing pseudogap in the attractive case. Observing antiferromagnetic correlations or superfluidity in 2D systems will require a further reduction in the entropy by a factor of three or more. It is possible that the inhomogeneous density in a trap can lead to a redistribution of entropy with some regions having a much lower entropy than others.

[1] M. Kohl *et al.*, Phys. Rev. Lett. **94**, 080403 (2005).
[2] J.K. Chin *et al.*, Nature **443**, 961 (2006).
[3] R. Jordens *et al.*, Nature **455**, 204 (2008).
[4] U. Schneider *et al.*, Science **322**, 1520 (2008).
[5] W. Hofstetter *et al.*, Phys. Rev. Lett. **89**, 220407 (2002).
[6] D. Jaksch and P. Zoller, Ann. Phys. **315**, 52 (2005); D. Jaksch *etal.*, Phys. Rev. Lett. **81**, 3108 (1998).
[7] D.J. Scalapino in "Handbook of High Temperature Superconductivity", edited by J.R. Schrieffer and J.S. Brooks, (Springer, 2007); arXiv:cond-mat/0610710.
[8] P.W. Anderson *et al.*, J. Phys. Cond. Mat. **16**, R755 (2004).
[9] T. Giamarchi, "Quantum physics in one dimension" (Oxford, 2004).
[10] A. Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996).
[11] J.E. Hirsch, Phys. Rev. B **28**, 4059 (1983).
[12] A. Moreo and D.J. Scalapino, Phys. Rev. Lett. **66**, 946 (1991).
[13] M. Randeria *et al.*, Phys. Rev. Lett. **69**, 2001 (1992); N. Trivedi and M. Randeria, Phys. Rev. Lett. **75**, 312 (1995).
[14] J.R. Schrieffer, X.G. Wen, and S.C. Zhang Phys. Rev. B **39**, 11663 (1989).
[15] M.S. Makivic and H-Q. Ding, Phys. Rev. B **43**, 3562 (1991).
[16] K. Binder, Z. Phys. **45**, 61 (1981).
[17] A.-M. Dare *et al.*, Phys. Rev. B **76**, 064402 (2007).
[18] T. Paiva *et al.*, Phys. Rev. B **63**, 125116 (2001).
[19] F. Werner *et al.*, Phys. Rev. Lett. **95**, 056401 (2005).

[20] D.J. Scalapino, S.R. White, and S.C. Zhang, Phys. Rev. B **47**, 7995 (1993).